Special Topics on Basic EECS I
VLSI Devices
Lecture 2

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1D space with a flat potential (Free electron)

- Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x)$$

  - Periodic boundary condition, $\psi(0) = \psi(Na)$.
  - Its solution

$$\psi(x) \propto \exp\left(i\frac{2\pi}{Na}nx\right) = \exp ikx$$

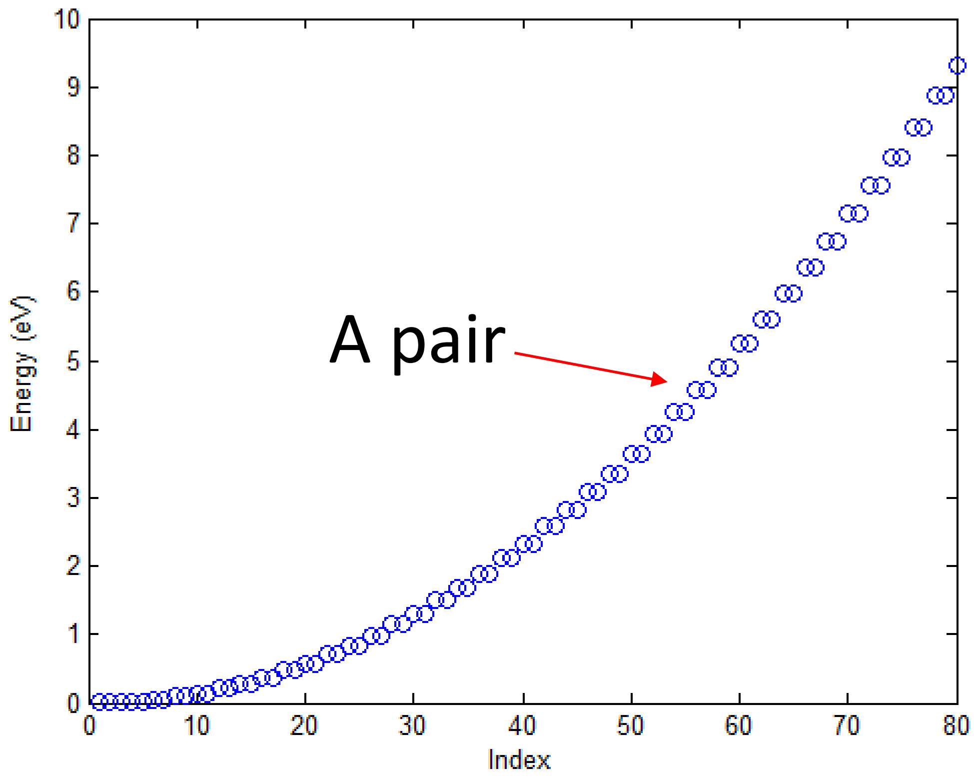
Plane wave

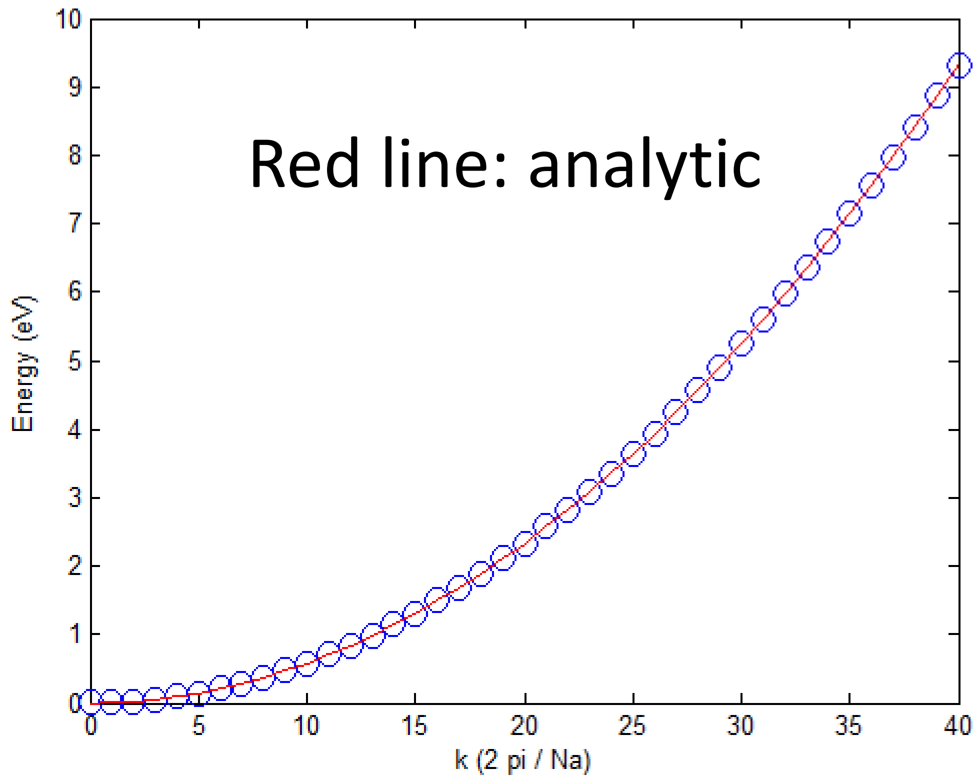
$$E = \frac{\hbar^2}{2m}k^2$$

  - k can be used to identify a state.

Numerical example (Free electron)

- When a is 0.4 nm and N is 40,
  - 80 states with lowest energies

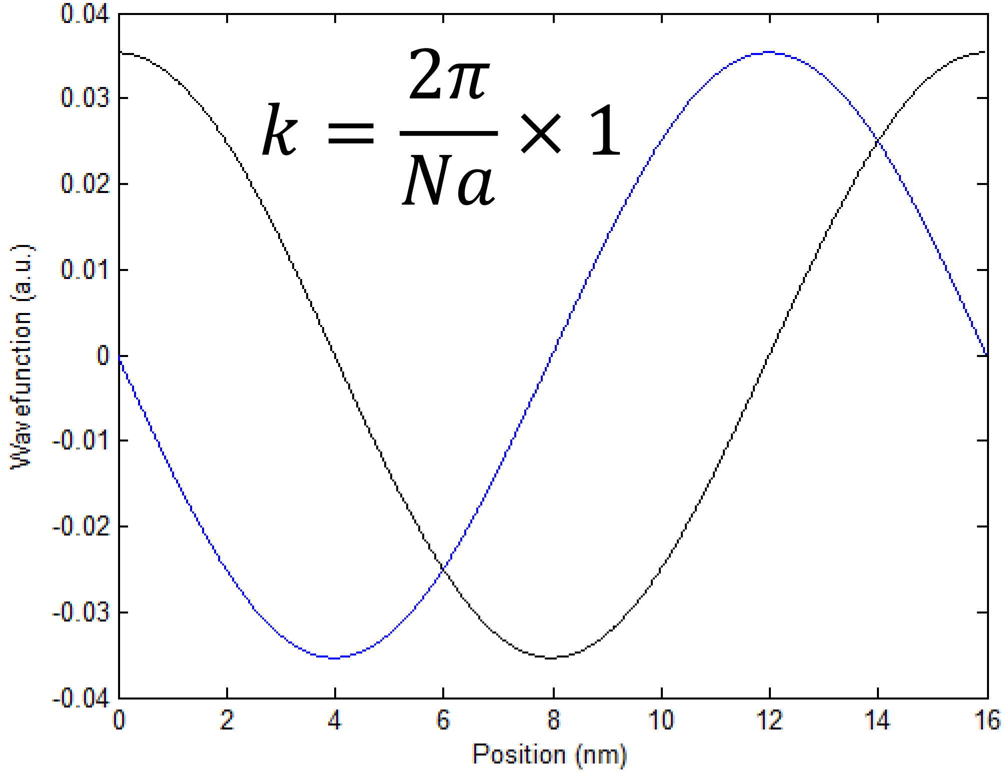


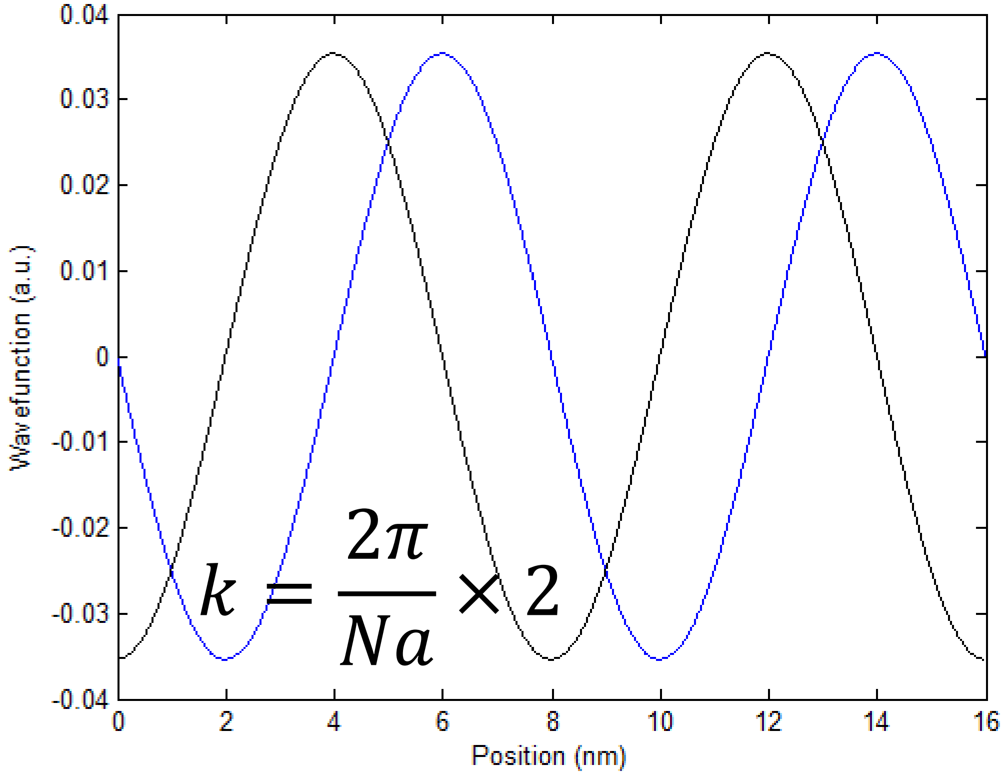


Pair?

- Two sinusoidal wavefunctions with the same period

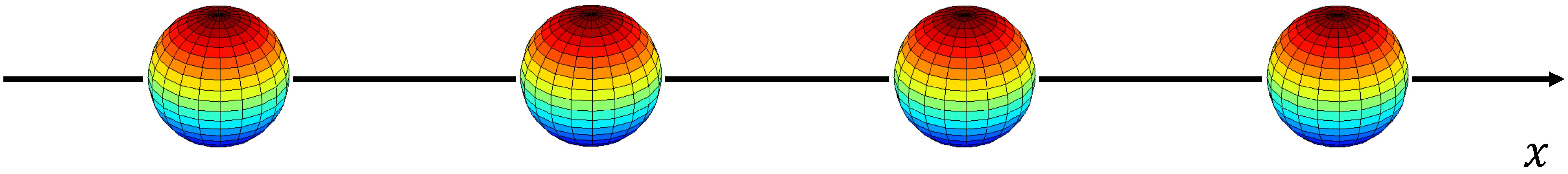
$$\exp ikx = \cos kx + i \sin kx, \exp(-ikx) = \cos kx - i \sin kx$$





Periodicity

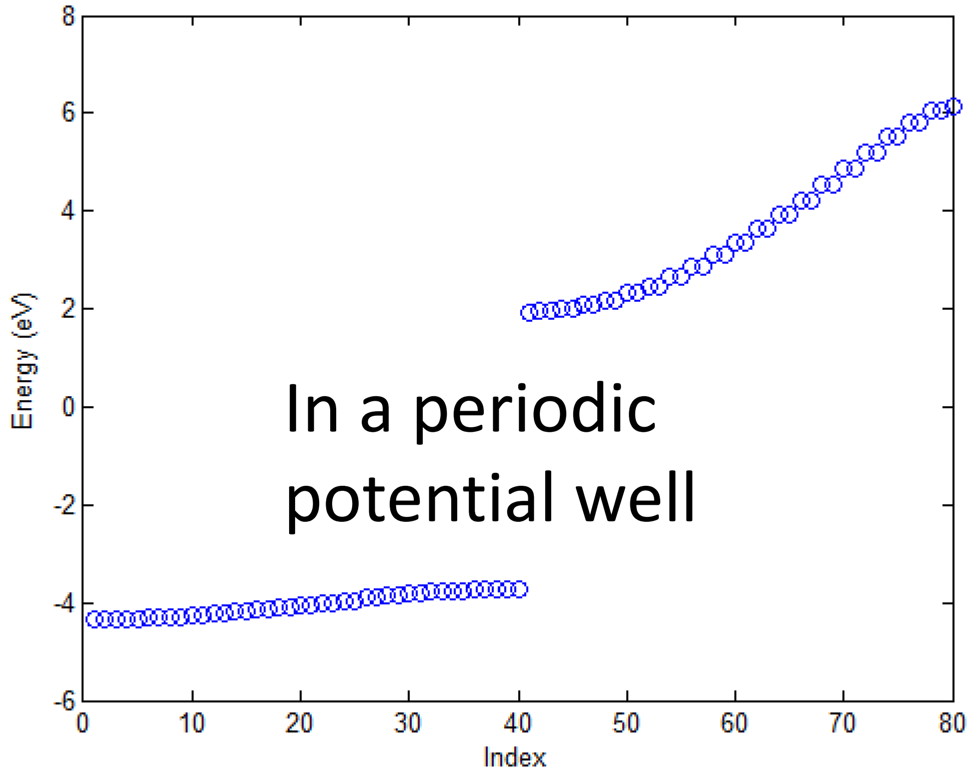
- Atoms are placed in a periodic manner.
  - They are attracting electrons. (Negative potential)

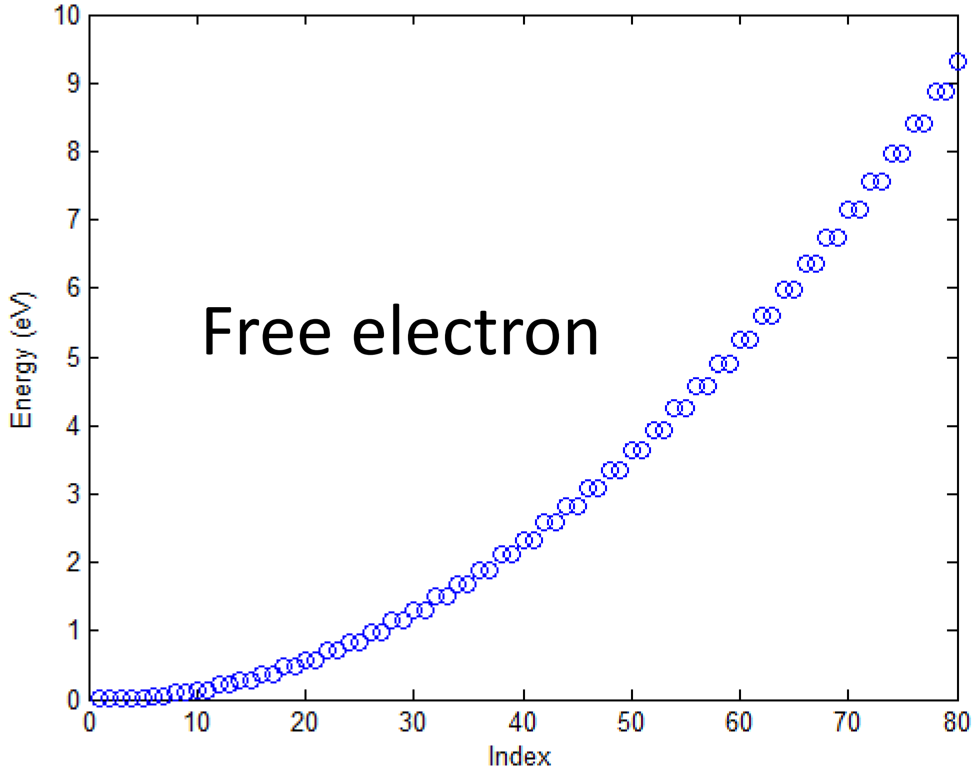


  - Let us consider a periodic potential well.

Numerical example (Periodic potential well)

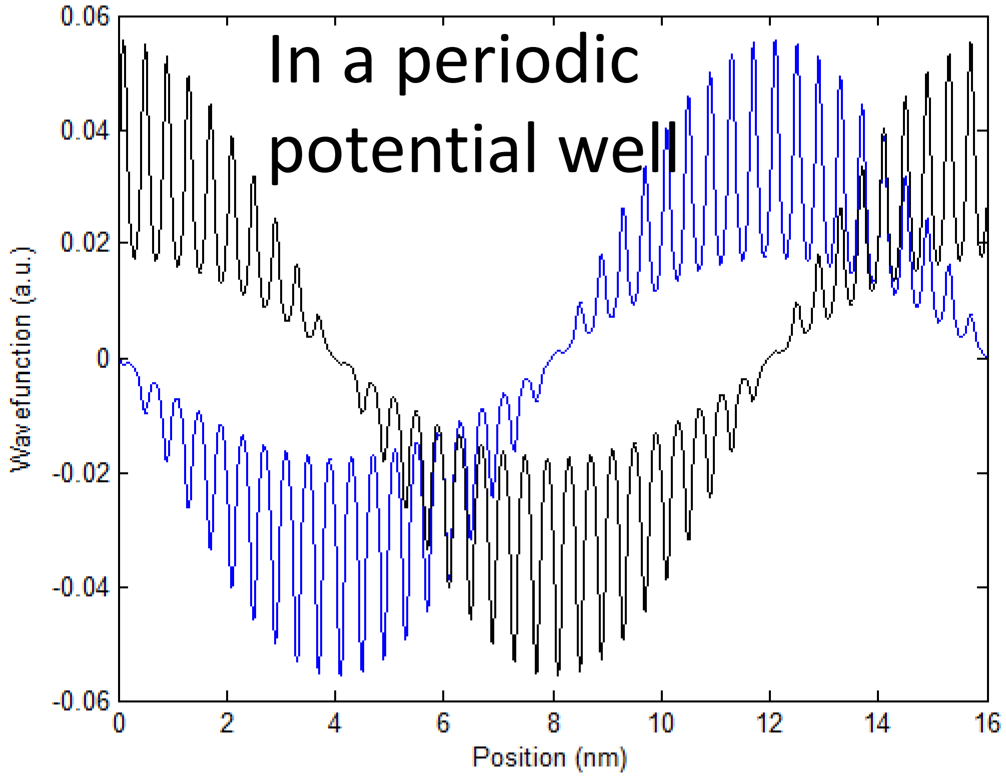
- When a is 0.4 nm, N is 40, the well width is 10 nm, and the well depth is 10.0 eV,

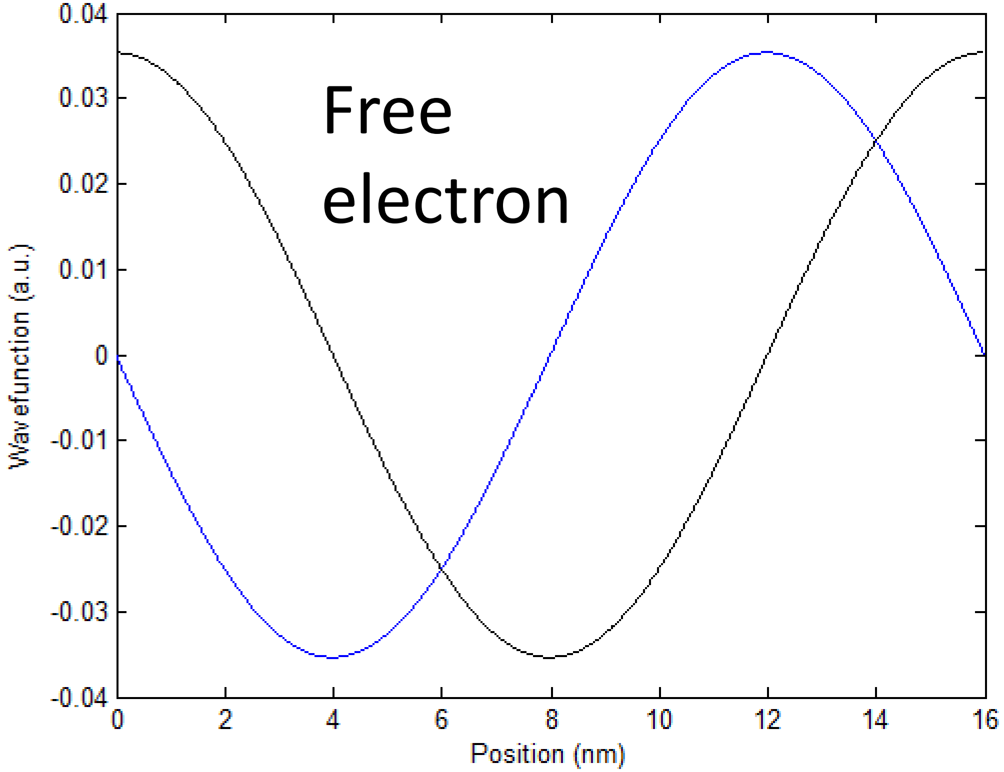




Wavefunction (Periodic potential well)

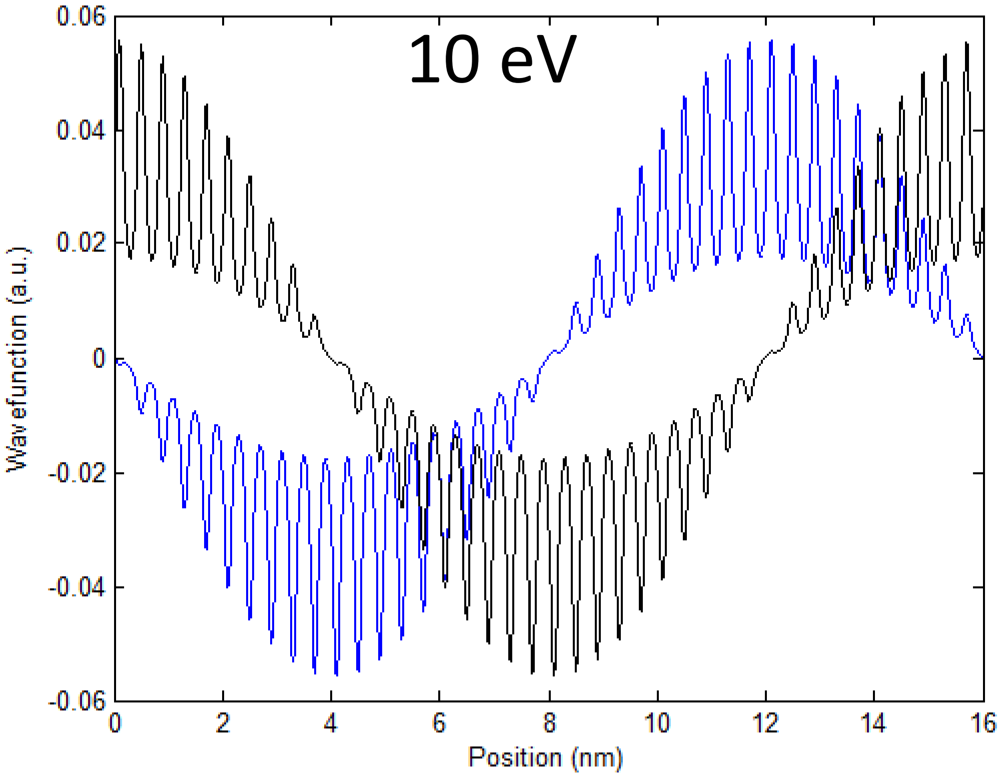
- When a is 0.4 nm, N is 40, the well width is 0.1 nm, and the well depth is 10.0 eV,

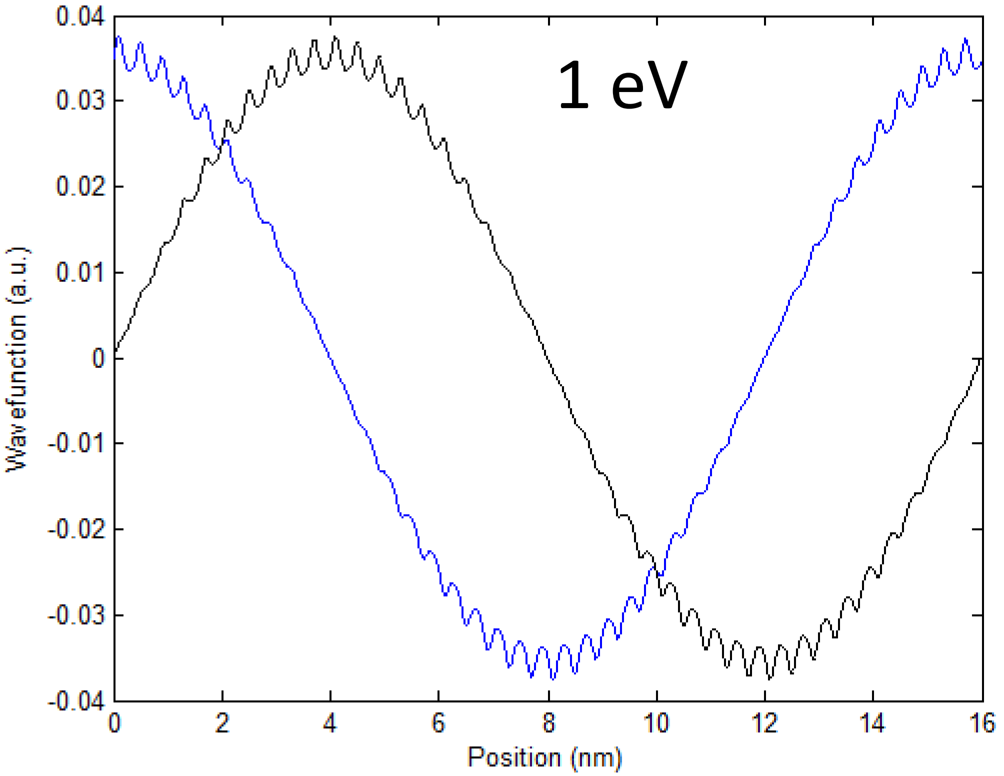




Observation

- $\psi(x)$ in a periodic potential well is a modulated version of the free electron wave function.





Bloch theorem

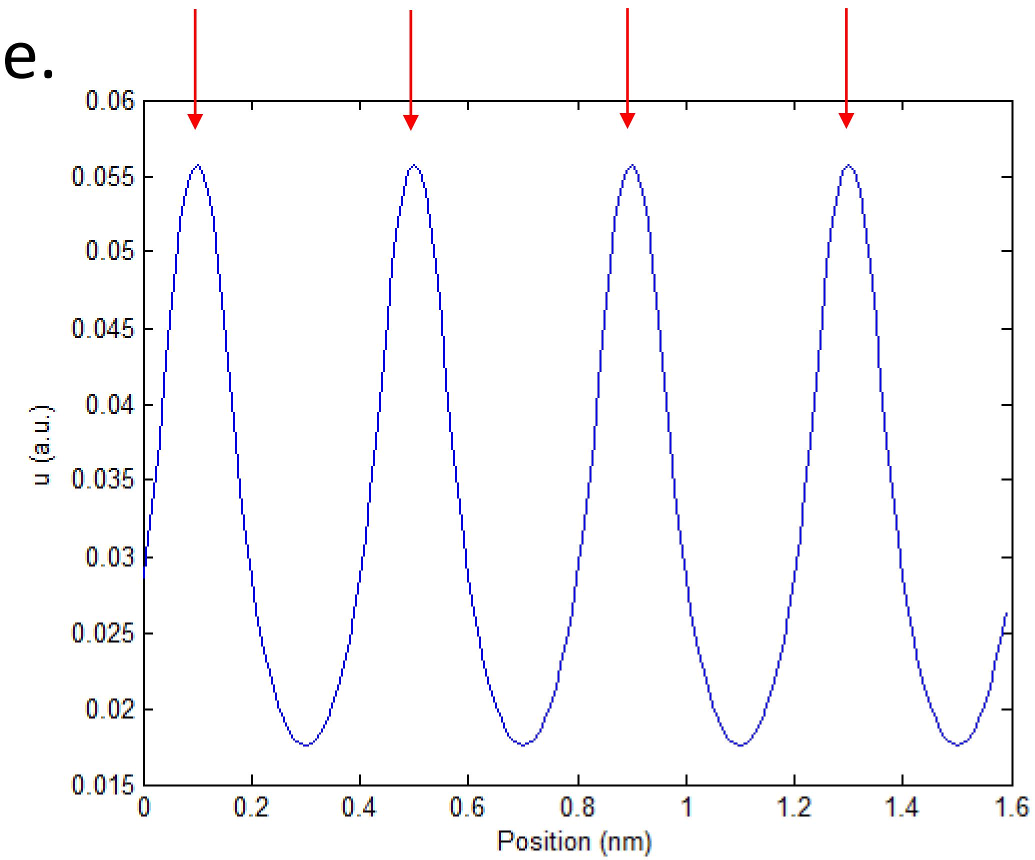
- Under a periodic potential, the wavefucntion can be expressed in a form of

$$\psi(\mathbf{r}) = u(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}$$

  - $u(\mathbf{r})$ is periodic within the direct lattice.

    $u(\mathbf{r}+\mathbf{R}) = u(\mathbf{r})$

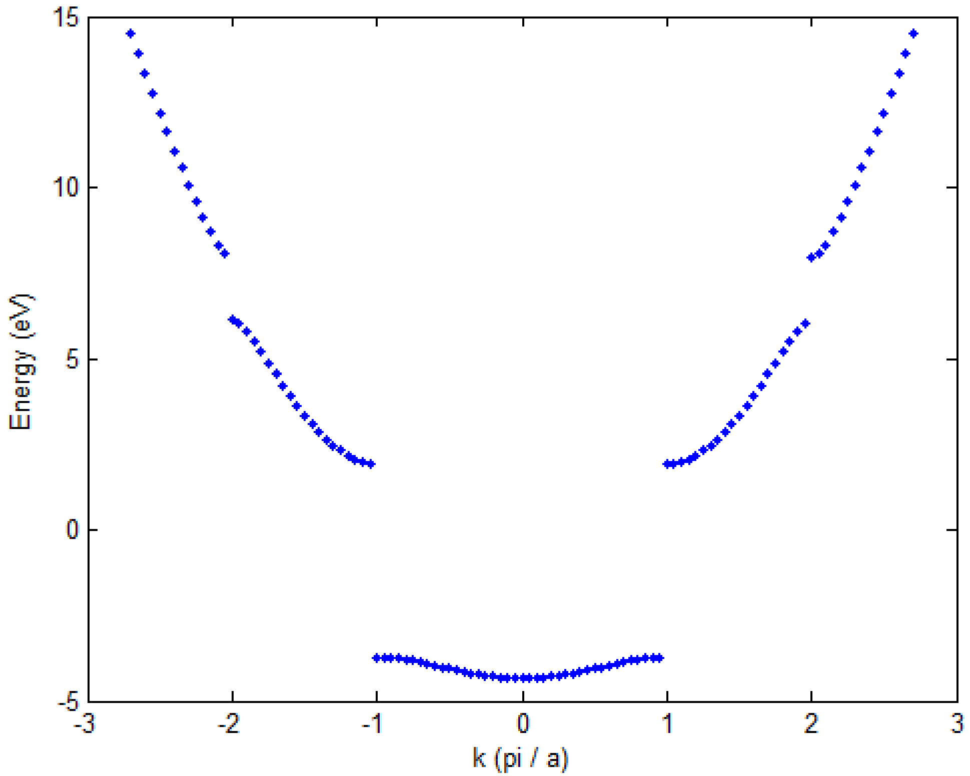
    $\mathbf{R} = i\mathbf{a}_1 + j\mathbf{a}_2 + k\mathbf{a}_3$
  - $\mathbf{k}$ can be used to identify a state, still.

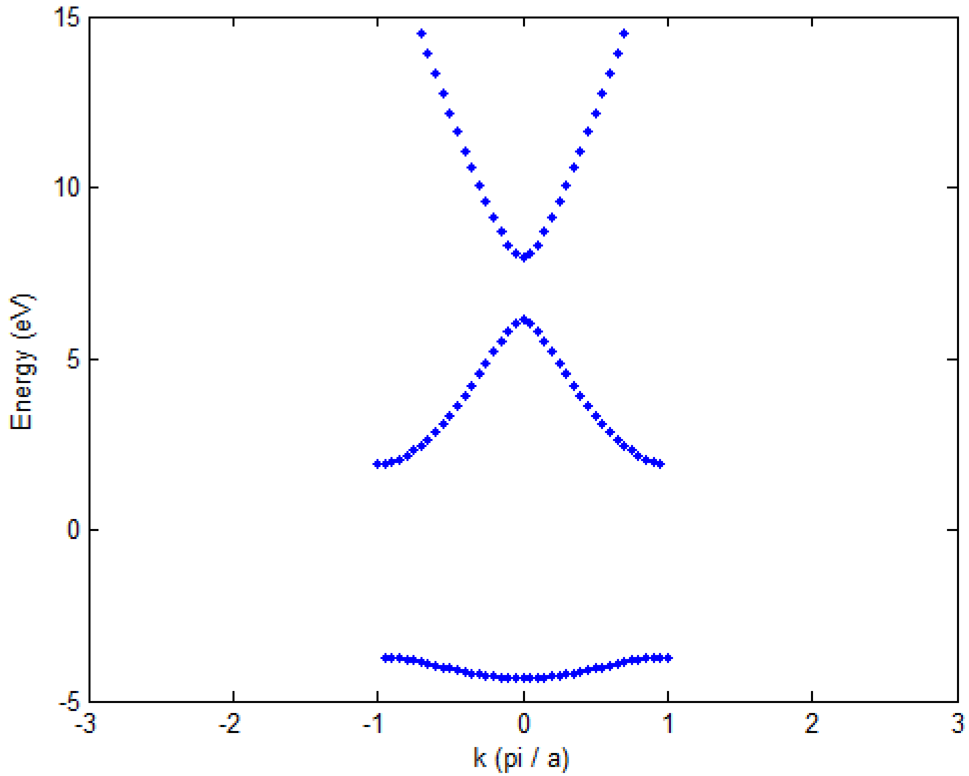


10 eV, $k = \frac{2\pi}{Na} \times 1$

Reduced zone scheme

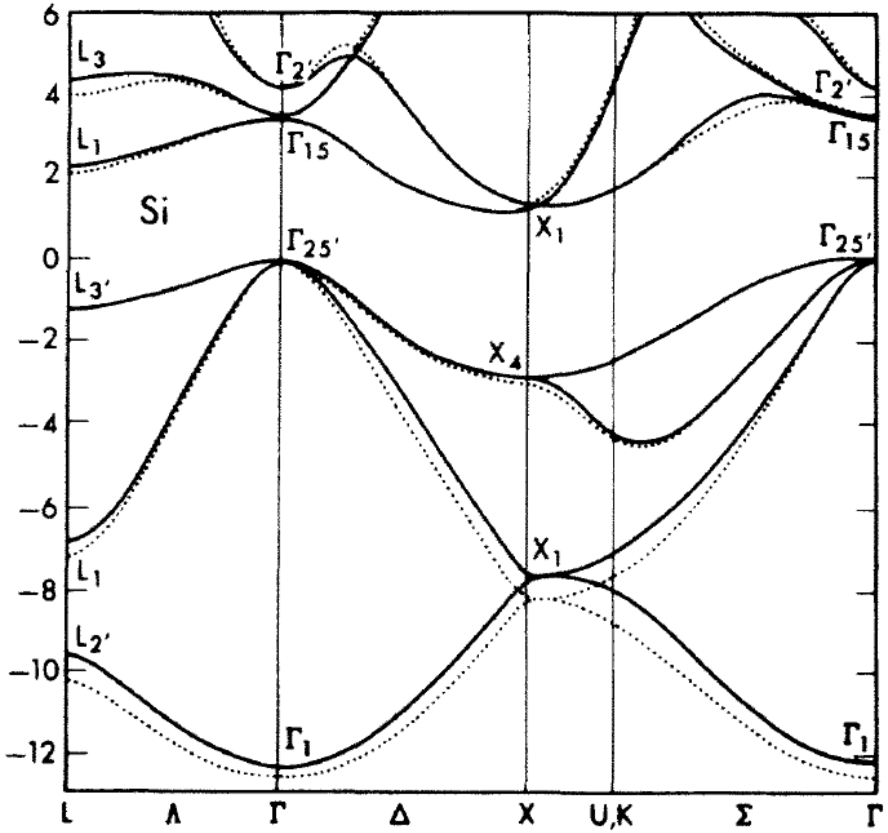
- When $\mathbf{k}$ is outside the first BZ, it is mapped onto the first BZ.

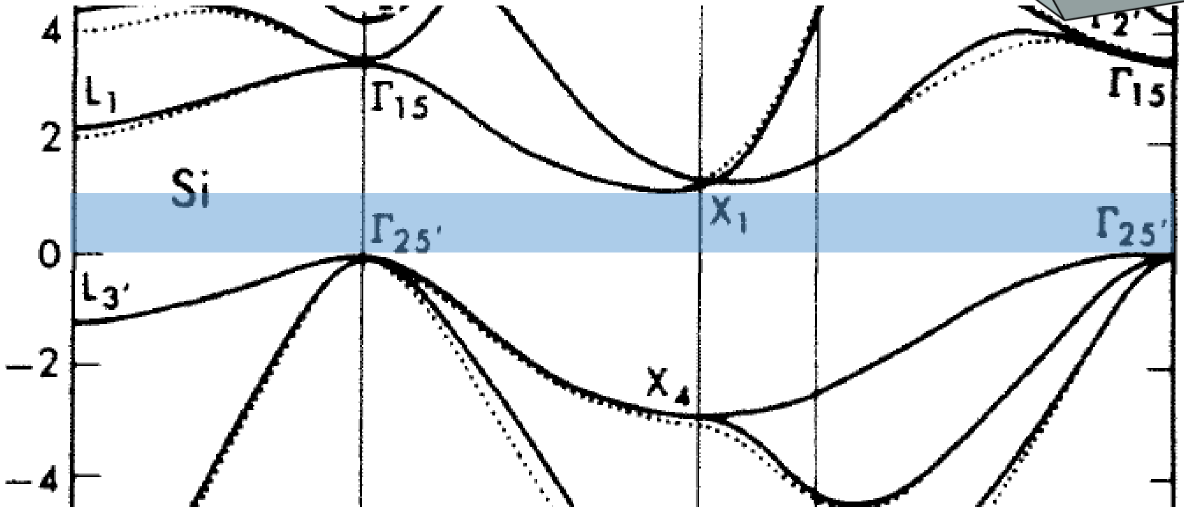


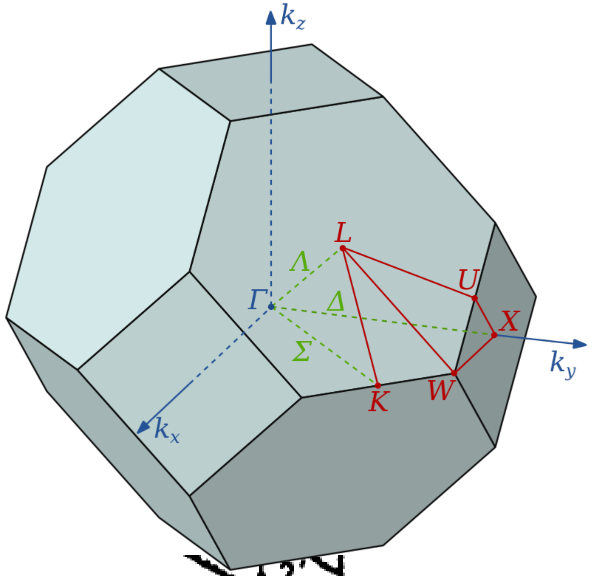


Band structure

- We can draw the $E - k$ diagram.
  - Bandgap is found.

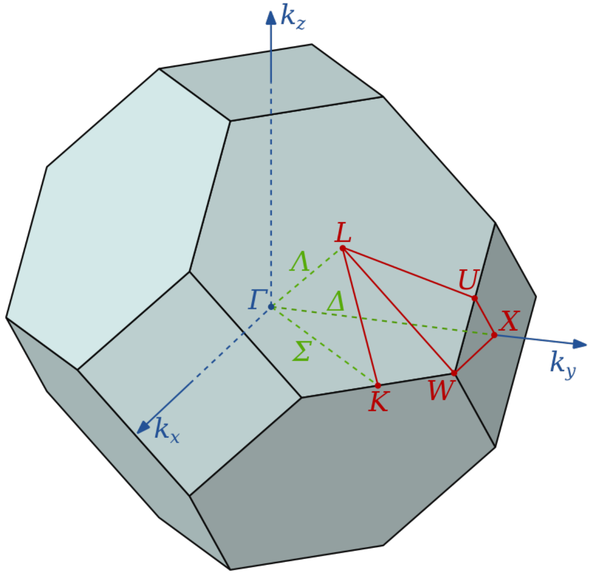






Silicon band structure
(Chelikowsky and Cohen, PRB, vol. 14, p. 556, 1976)

Velocity and inverse mass



- Velocity

$$\mathbf{v}(\mathbf{k}) = \frac{1}{\hbar}\nabla_k E(\mathbf{k})$$

- Inverse mass (its ij component)

$$m_{ij}^{-1} = \frac{1}{\hbar^2}\frac{\partial}{\partial k_i}\frac{\partial}{\partial k_j}E(\mathbf{k})$$

- Example) Silicon conduction band

$$E(\mathbf{k}) - E_c = \frac{\hbar^2}{2}\left(\frac{1}{m_{xx}}k_x^2 + \frac{1}{m_{yy}}k_y^2 + \frac{1}{m_{zz}}k_x^2\right)$$ ~ Taur, Eq. (2.2)

  – Among three masses, one is m_l and the other two are m_t.

Thank you!